Development of transport/inversion algorithms and capabilities for countermeasures to chem/bio/rad attacks in support of homeland security

SAND2004-1190P

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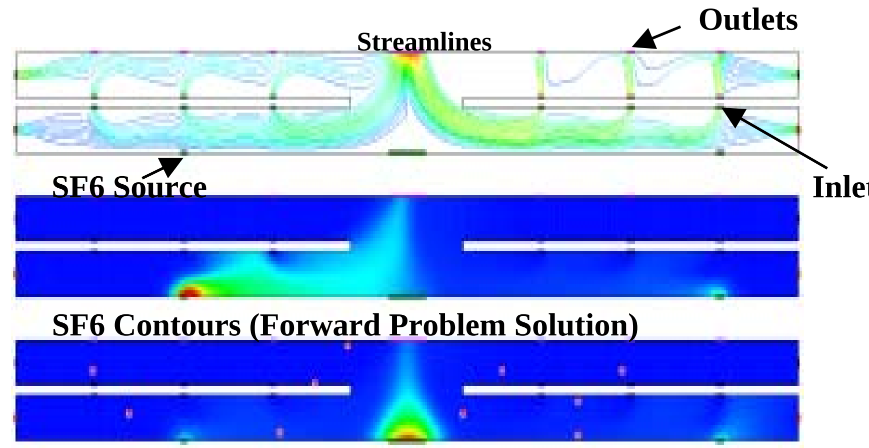
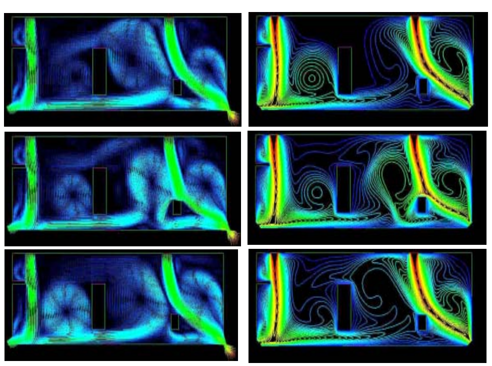
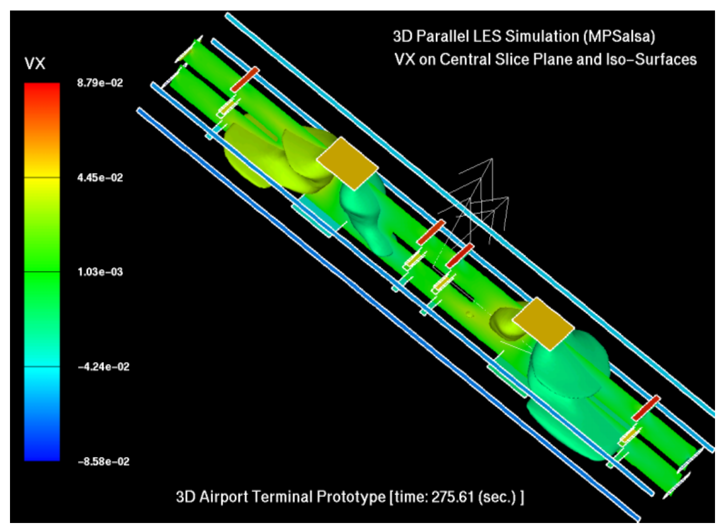


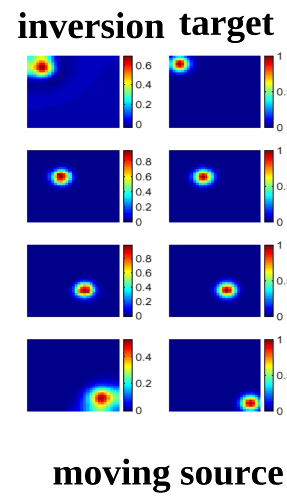
Setup for Optimization Problem: Locations of 10 sensors, SF6 contours at initial guess

Preliminary Decontamination Simulation: Transient Infusion of $Cl0_2$, H_2O to Neutralize Anthrax



Velocity Vectors ClO_2 Contours





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Outline

- **Motivation**
- **Describe Project Focus on General Transport / Inversion Technology**
- **A Brief Overview of Transport Models & Performance and Example Results**
- **A Brief Overview of the Source Inversion Formulation and Implementation**
- **An Example of Transport / Reaction Modeling applied to Decontamination**
- **Leveraged Efforts**
- **Major Next Steps**

Motivation: Transport/Inversion/Optimization Algorithms Can Contribute to all Phases of a DHS Level Event*

Event Phases	Corresponding activities/required capabilities
Pre-event	♦ Vulnerability and risk analysis for sites/infrastructure ♦ Sensor/surveillance design/evaluation R&D capabilities ♦ Sensor/surveillance network architecture and sensor placement studies ♦ Planning for response to disasters/accident/attack events, …. Etc.
Event	♦ Process sensor/surveillance alerts (fusion of sensor data / simulation modeling) ♦ Characterize accident/attack (Chem-Bio, explosives, RadNuc, etc.) ♦ Estimate source location of accident/attack if unknown ♦ Provide real-time predictions of consequences of CBRN accident/attack ♦ Select and execute planned mitigation strategies, …. Etc.
Post-Event	♦ Execute containment or control strategies if applicable ♦ Refine characterization of accident/attack if unknown (source identification, source location, source reconstruction, etc.) ♦ Begin forensics and attribution efforts. …. Etc.
Remediation/ Decontamination	♦ Plan remediation effort ♦ Execute remediation - monitor, evaluate and adaptively guide effort ♦ Perform evaluation and initiate new Pre-event planning effort, … Etc.

- Adapted from draft report ASC / DHS workshop (Oct. 2003) – High Level Simulation Strategies (J. Shadid and G. Sugiyama)
- activities/capabilities called out by (CIP, BTS, EP&R, TVTA, Chem-Bio, RadNuc) DHS ASC Workshop speakers/sessions

A Focus on Development of General Transport and Inversion Technology - Demonstrated on Internal Flows (applies to External)

Current Demonstration Codes to Prototype Strategy & Algorithms

- Mpsalsa* (flow/transport/reactions)
- MOOCHO/rSQP++
  (PDE Constrained Optimization)
- Dakota (black-box Optimization)

* This work was partially supported by the DOE/SC MICS Applied Mathematical Sciences program

Technical Issues (project plan):

- Flow / Transport Modeling and Solution Methods
    - Turbulence modeling
    - Particle transport Formulations (Eulerian/Lagrangian)
    - Scalable Efficient Solvers
- Algorithms for Source Inversion
    - Optimization techniques (PDE Constrained)
    - Transient analysis
    - Uncertainty and reliability (sensors)
- Algorithms for Optimal sensor placement
- Evaluation of Operational models (real time):
    - Development and critical evaluation of
        - Hierarchical Physics Based Models
        - Nonlinear Reduced Order Modeling (ROM)
    - Verification with high fidelity models
    - Uncertainty quantification
- High Fidelity Operational models for Pre-event/Post-event

Important additional issues:

- Decontamination/remediation with reacting flow modeling
- Control – Optimization Methods (HVAC)
- Forensic studies using simulation and source reconstruction
- Adaptive contaminant sampling strategy using simulation
- …..

High Fidelity Chemically Reacting Flow Solver (MPSalsa)

Governing Equation	Flow and Transport PDE Residuals
Momentum	$\mathbf{R_m} = \rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \bullet \nabla \mathbf{u}) - \nabla \bullet \mathbf{T} - \rho \mathbf{g}$
Total Mass	$R_p = \frac{\partial \rho}{\partial t} + \nabla \bullet (\rho \mathbf{u})$
Thermal Energy	$R_T = \rho \hat{C}_P \left[\frac{\partial T}{\partial t} + \mathbf{u} \bullet \nabla T \right] + \nabla \bullet \mathbf{q} - \Theta - \dot{Q} + \sum_{k=1}^{N} \mathbf{j_k} \bullet \hat{C}_{P,k} \nabla T - \sum_{k=1}^{N} h_k W_k \dot{\omega}_k$
Species Mass Fraction for Species k (k =1,2,….,N-1)	$R_{Y_k} = \rho \left[\frac{\partial Y_k}{\partial t} + \mathbf{u} \bullet \nabla Y_k \right] + \nabla \bullet \mathbf{j}_k - W_k \dot{\omega}_k$

Turbulence Eq(s). PDE residuals

k-ε model

$$\frac{\partial \bar{\rho} k}{\partial t} + \frac{\partial}{\partial x_j}\left[\bar{\rho}\tilde{u}_i k\right] = \bar{\rho}\mathbf{P} - \bar{\rho}\varepsilon + \frac{\partial}{\partial x_j}\left(\left(\bar{\mu} + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right)$$

$$\frac{\partial \bar{\rho} \varepsilon}{\partial t} + \frac{\partial}{\partial x_j}\left[\bar{\rho}\tilde{u}_i \varepsilon\right] = C_{\varepsilon 1}\bar{\rho}\mathbf{P}\frac{\varepsilon}{k} - C_{\varepsilon 2}\bar{\rho}\frac{\varepsilon^2}{k} + \frac{\partial}{\partial x_j}\left(\left(\bar{\mu} + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right)$$

$$\mathbf{P} = \tau_{ij}\frac{\partial \tilde{u}_i}{\partial x_j}$$

Spalart-Allmaras model

$$\frac{\partial \bar{\rho}\hat{\upsilon}}{\partial t} + \frac{\partial}{\partial x_j}\left[\bar{\rho}\tilde{u}_i\hat{\upsilon}\right] = C_{b1}\bar{\rho}\hat{\upsilon}\hat{S} - C_{w1} f_w \bar{\rho}\left(\frac{\hat{\upsilon}}{d}\right)^2 + \frac{\partial}{\partial x_j}\left(\frac{\bar{\mu} + \bar{\rho}\hat{\upsilon}}{\sigma}\frac{\partial \hat{\upsilon}}{\partial x_j}\right) + \frac{C_{b2}\bar{\rho}}{\sigma}\frac{\partial \hat{\upsilon}}{\partial x_j}\frac{\partial \hat{\upsilon}}{\partial x_j}$$

Smagorinsky eddy viscosity model (Constant and Dynamic Model)

$$\nu_t = C_S \bar{\Delta}^2 \left(2\bar{S}_{ij}\bar{S}_{ij}\right)^{1/2}$$

Subgrid kinetic energy eddy viscosity model (Schumann, Kim and Menon)

$$\rho\frac{\partial ksgs}{\partial t} + \rho\mathbf{u} \bullet \nabla ksgs + \mathbf{P} - \mathbf{D} - \nabla \bullet \left(\nu_t \nabla ksgs\right) = 0$$

$$\nu_t = C_\nu \bar{\Delta}\left(ksgs\right)^{1/2} \qquad \tau_{ij}^{sgs} = -2\nu_t \bar{S}_{ij} + \frac{2}{3}\delta_{ij} ksgs$$

A Brief Summary of the Formulation, Numerical Methods and Software

- Spatial Discretization: 2D/3D linear and quadratic unstructured FE. (Quad/Hex and Triangle/Tets)
- FE Formulation: Stabilized Finite Element Formulation (Hughes et. al., Shakib, Tezduyar, Franca)
- Parallel Formulation: Nodal based decomposition (**Chaco**), unstructured communication (MPI & **Aztec**)
- Time Integration: Predictor/corrector & error control, 1^{st} to 2^{nd} order methods.
- Nonlinear Solver: Inexact Newton method (Eisenstat and Walker; Shadid, Tuminaro and Walker)
- Optimization: Multi-parameter optimization, black-box (**Dakota** – Eldred et. al.),

  PDE constrained Optimization (**MOOCHO**, **TSFcore** -Bartlett, van Bloemen Waanders**)**
- Linear Solvers: Parallel Krylov methods with domain decomposition and multi-level preconditioners

  (Aztec/ML; Tuminaro, Shadid, Hutchinson, Tong, Sala…)

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Inter-relationship of models for flow and transport in large-scale structures.

Incompressible Flow Models:

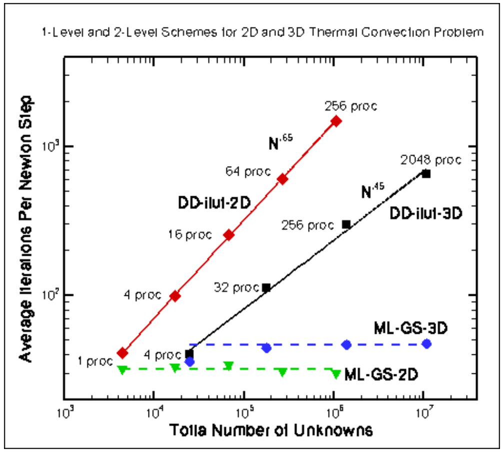
- **High Fidelity Models (Stabilized FEM)**
  - **Reynolds Averaged Navier-Stokes (RANS)**
    Mean steady approximation
    Transient flow
  - **Large Eddy Simulation (LES)**
    Time averaged steady
    Transient flow

High fidelity used to verify lower fidelity

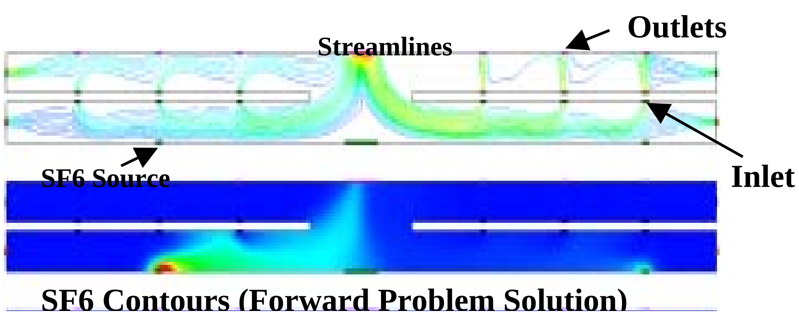
- **Lower Fidelity Models**
  - **Zonal Models of large structures with many small rooms Collaborators (Restoration DDAP)**
- **Operational Models – real time**
  - **Hierarchical physics based**
    Collab, (External flow – NARAC)

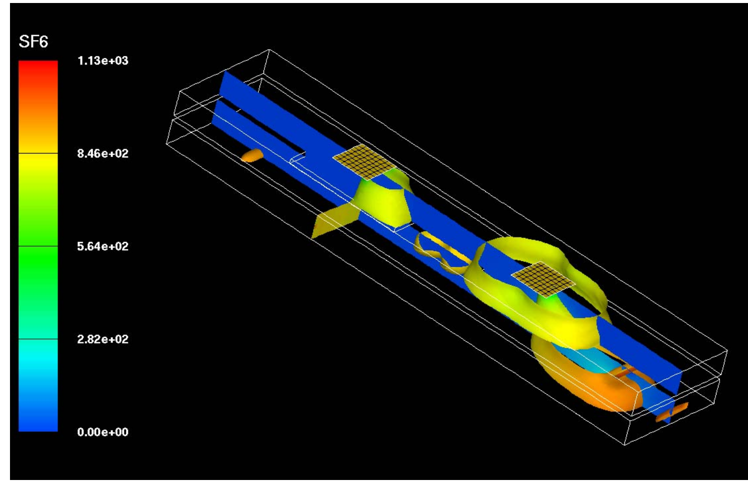
High fidelity used to develop ROM

  - **Reduced order modeling methods (POD, CVT) use off line high fidelity computations**



2D and 3D steady laminar* flow transport results





	method	smoothers/ solvers	fine mesh unknowns	its per newton step	time (sec)	hardware
2D	1-level DD	ilu	619,300	500 [10]	10,460	20 1-GHz P3
	2-level geom	ilu-superlu	619,300	17 [7]	118	20 1-GHz P3
	2-level geom	ilu-superlu	9.8M*	293 [7]	3266	128 nodes cplant
3D	1-level DD	ilu	872,000	118 [7]	1801	16 1-GHz P3
	2-level geom	ilu-superlu	872,000	21 [6]	795	16 1-GHz P3
	2-level geom	ilu-superlu	28.9M*	40 [7]	5536	256 nodes cplant

* **Not run at turbulent operating conditions so direct to steady-state is possible, can be used as initial guess for steady RANS solution**

***1 –level did not converge**

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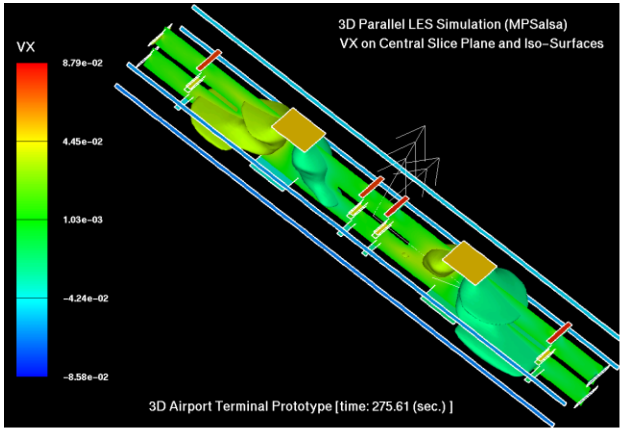
Comparison of methods: Turbulent transient LES

- 3D airport terminal prototype
  - **3.3M nodes (13.1M unknowns)**
- 1000 nodes Sandia Cplant machine (1 – GHz procs)

Turbulent Flow (LES) and Chemical Species Transport in 3D Prototype Airport



method	smoothers/ solvers	nodes per aggregate	coarse level unknowns	medium level unknowns	its per newton step	time per newt step (sec)
1-level DD	ilu				113	150
2-L geom	ilu-gmres/ilu		32336		24	255
2-L geom	gs2-gmres/ilu		32336		did not converge	
2-L AMG	ilu-superlu	512	19948		failed (mess pass err)	
3-L AMG	gs-ilu-superlu	100	1292	129444	31	38
3-L AMG	gs-ilu-superlu	512	44	20376	56	53

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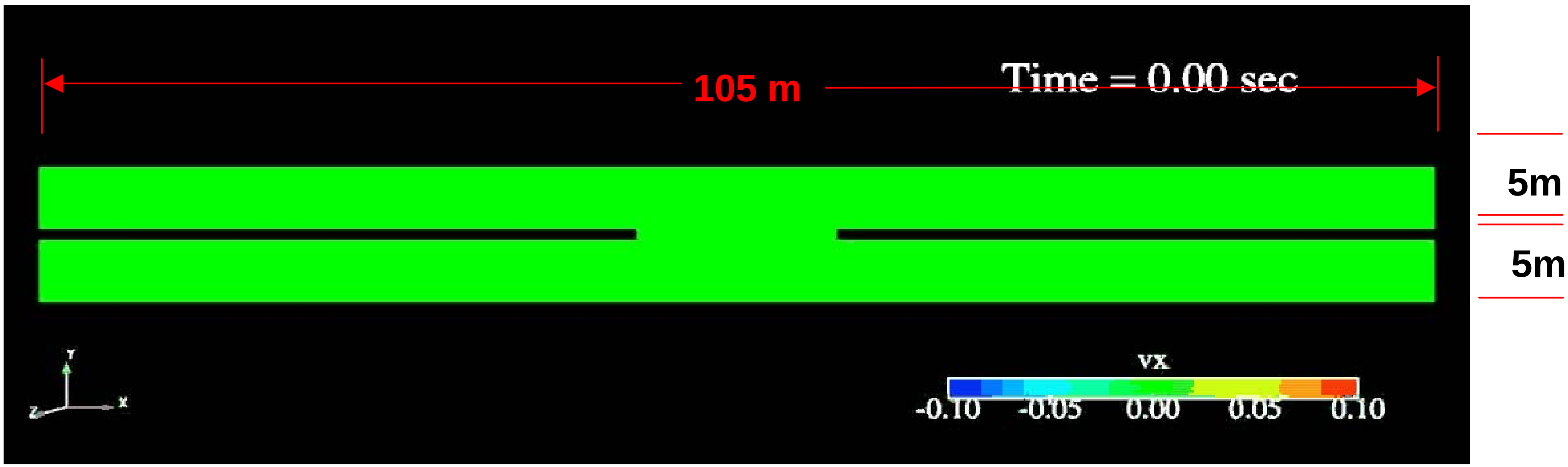
Flow in 2D Airport Terminal Prototype: Transient LES-ksgs Turbulence Simulations



Max Vx = 0.245 m/s
Min Vx = -0.266 m/s

Model Information:
- 609,792 2D Quad elements
- 2.45M unknowns (u,v,P,ksgs)
- 1000 time steps (~ 1 sec. each CFL ~ .3)

Solver:
3 level - block aggregation AMG
(Gauss-Seidel, ILU, superlu)
- 42 sec. Per time step
- 19.4 hours total on 64 – 3 GHz procs.

MPSalsa

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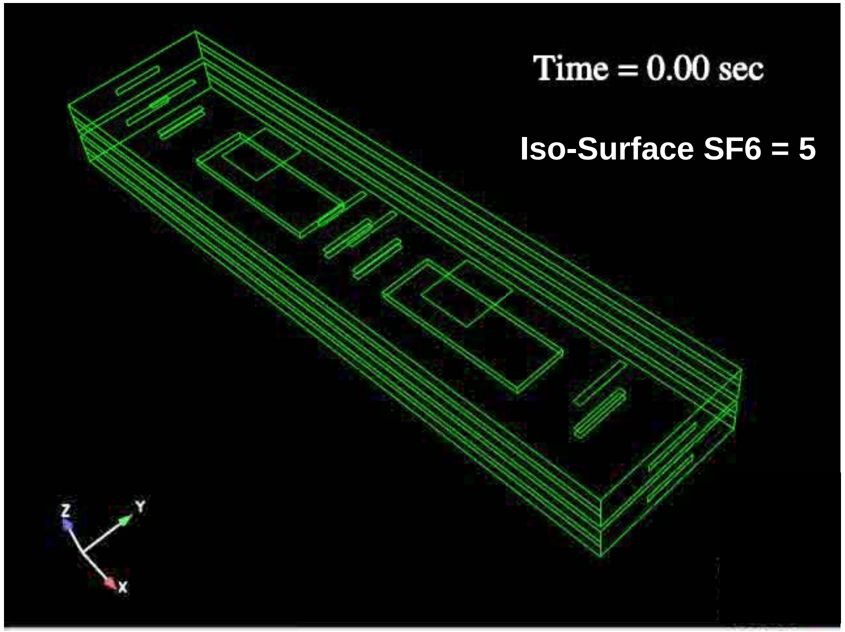
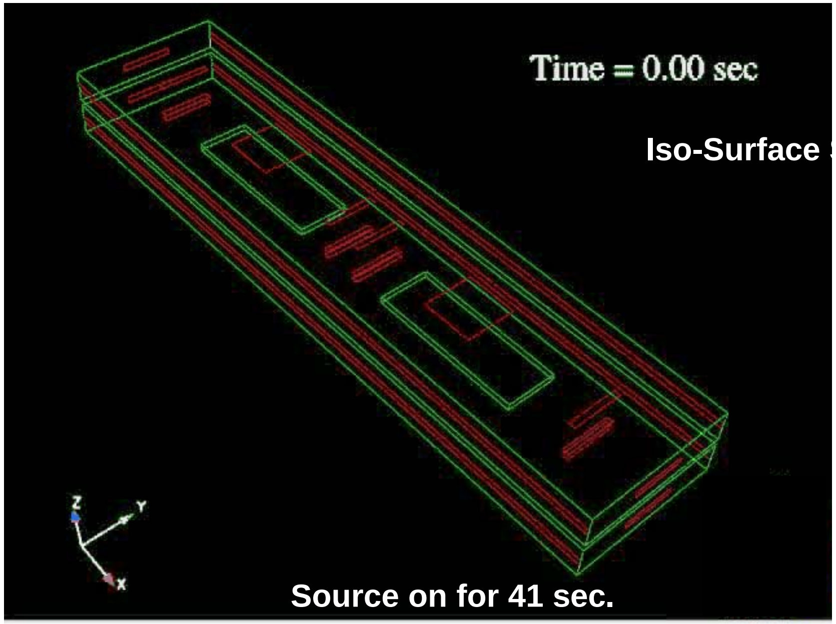
Transport Simulations for Chemical Attack in an Prototype Airport Terminal (Precomputed Steady turbulent Flow Field Approximation Constant Coeff. LES)

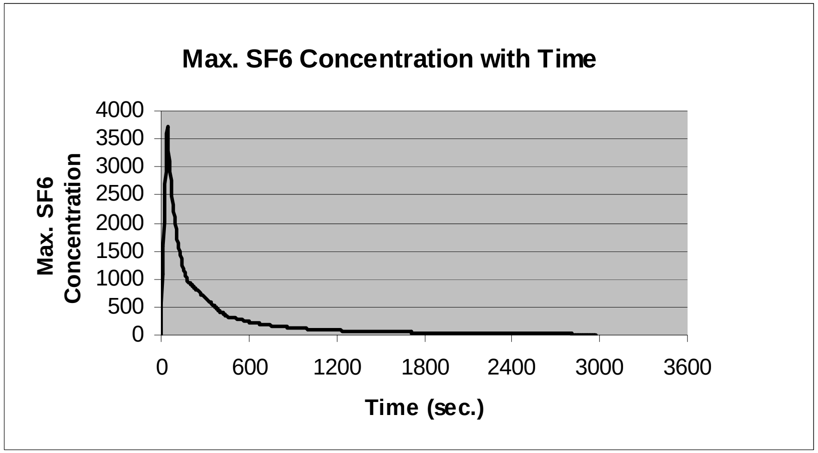




Chemical Transport Simulations

Size:
- **>.33M 3D Hex Element FE mesh**
- **>.33M SF6 Concentration Unknowns**

CPU time (1 GHz processors):
- **5 sec. time step @ ~4.6 sec on 16 procs.**



Source Inversion Formulation using PDE Constrained Optimization (SAND method)

$$\begin{array}{ll} \min\limits_{y,u} & f(y,u) \\ \text{s.t.} & c(y,u) = 0 \end{array}$$

$$\min_{f,c} \mathcal{J}(c,f) := \frac{1}{2}\sum_{j=1}^{N_r}\int_0^T s((c-c^*)^2, \delta(\boldsymbol{x}-\boldsymbol{x}_j))\,dt + \frac{1}{2}\beta\,\mathcal{R}(f),$$

$$\frac{\partial c}{\partial t} - k\Delta c + \nabla c \cdot \boldsymbol{v} + f = 0 \quad \text{in} \quad \Omega \times (0,T),$$

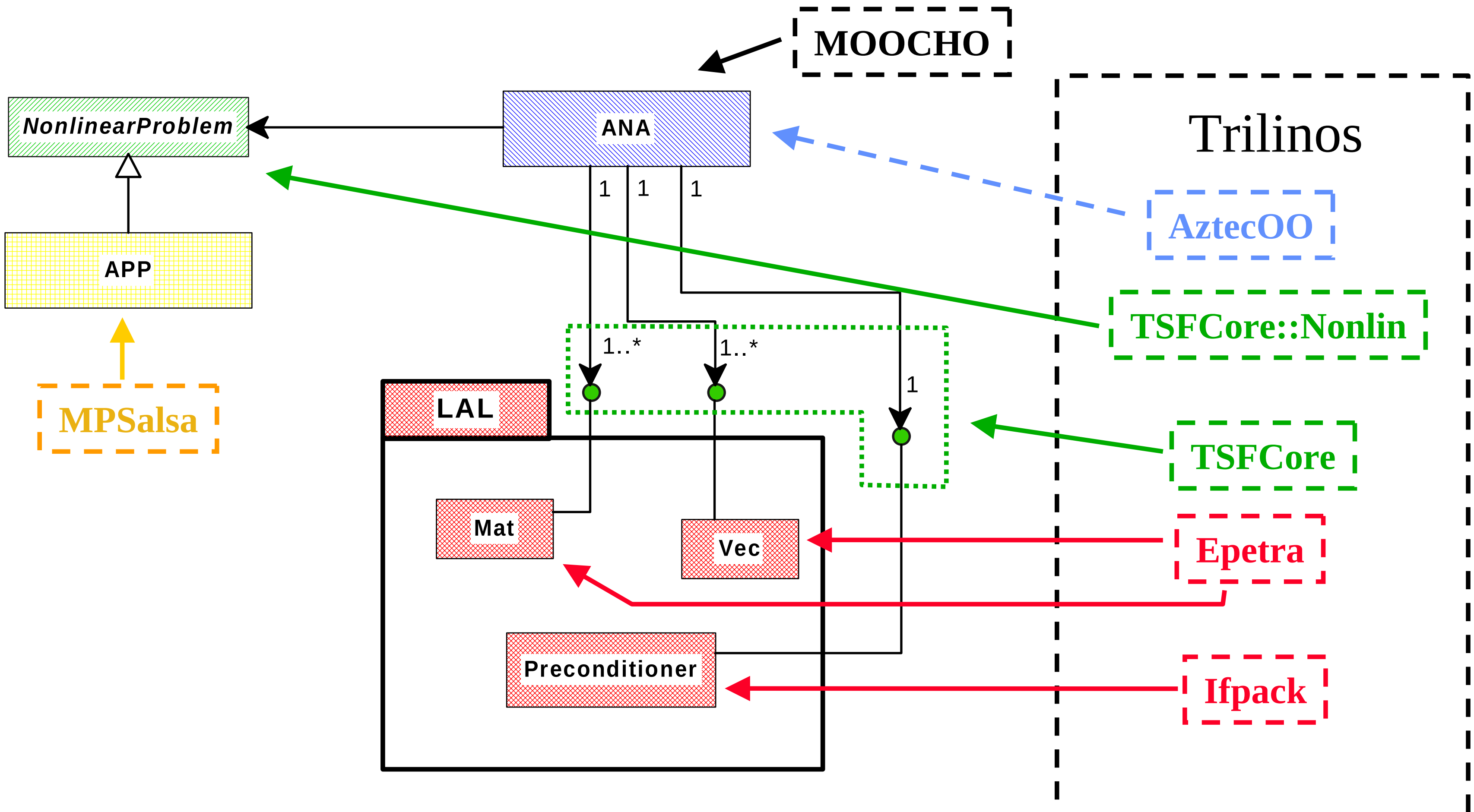
$$\frac{\partial c}{\partial n} = g \quad \text{on} \quad \Gamma_N \times (0,T), \qquad c = 0 \quad \text{on} \quad \Gamma_D \times (0,T),$$

$$c = c_0 \quad \text{in} \quad \Omega \quad \text{at} \quad t = 0,$$

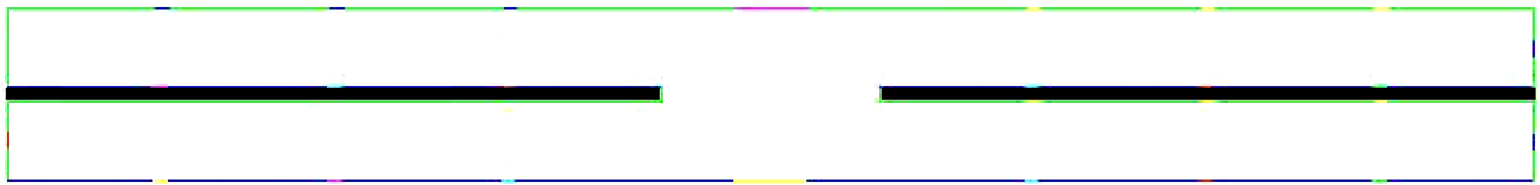
C* **- sensor values**
R **- regularization term to handle ill-conditioning of inverse problem**

Conv.-Diff. transport prob.

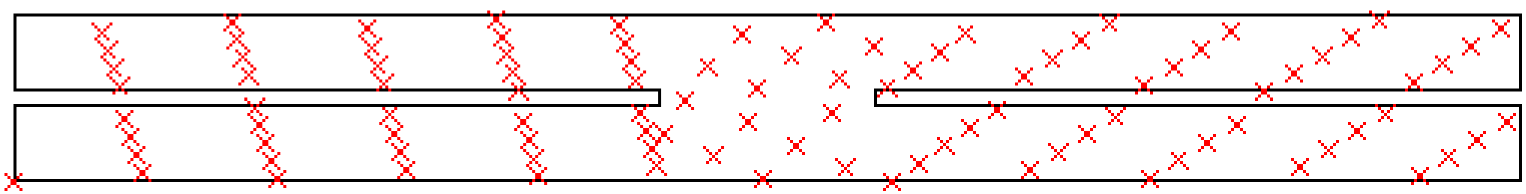
Parallel Source inversion using Production simulation code : MOOCHO / Trilinos / MPSalsa

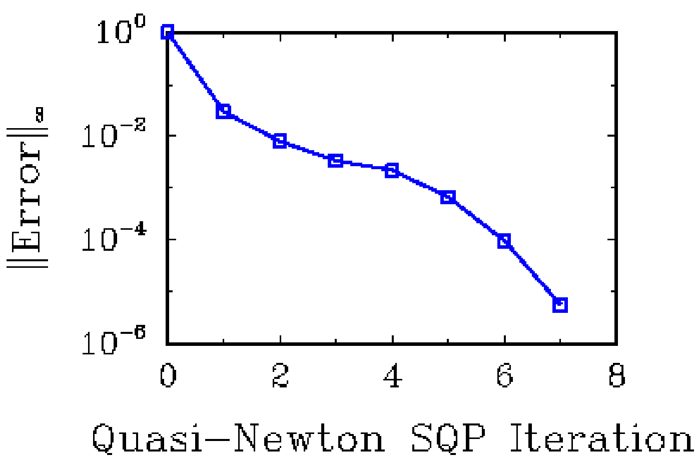


A Preliminary Verification of Steady Source Inversion Capability:
rSQP Quasi-Newton Approach (SAND Approach)



Set	0.0	0.0	1.0	0.0	0.0	0.0	0.1	0.0
Final	-7.7e-7	3.4e-6	0.999995	-5.6e-6	4.0e-6	-9.4e-7	0.1000002	2.7e-6





Details: (rank 2 BFGS)

- 55256 Concentration Unknowns (Flow -RANS Spallart-Almaras Model)
- 100 Sensors (similar accuracy with 55)
- 8 Inversion Parameters
  - Init = 0.0; Min = –0.01; Max = 2.0
- Inversion Details
  - 60 sec. On 16 Processors
  - 7 Quasi-Newton Iterations

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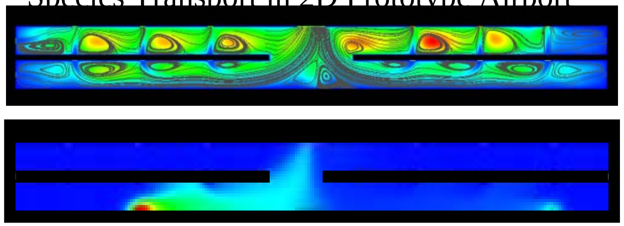
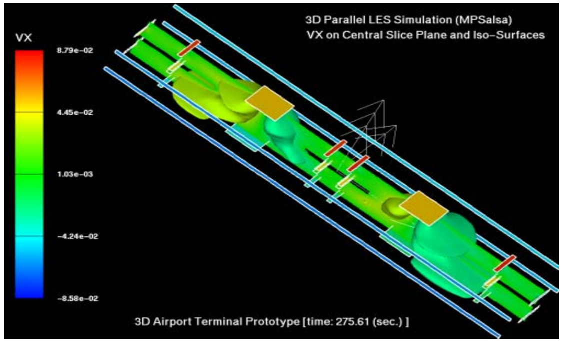
Preliminary Steady Source Inversion Capabilities 2D & 3D
10 – 1000 Inversion Parameters

Model	# Unknown Concentrations	# Inversion Parameters	CPU Time (sec.)		Hardware Procs - speed
			Offline	Online	
2D rSQP	55,356	8	-----	60	16 – 3 GHz
	55,356	100	----		
2D Precomputed Direct Sensitivities rSQP	55,356	500	3602	.44	4 – 2.4 GHz
	55,356	1000	6902	1.23	4 – 2.4 GHz
3D rSQP	.33M	8	----	720	16 – 3 GHz
	.33M	100			
3D Precomputed Direct Sensitivities rSQP (55 Sensors)	.33M	100	1680	7.3	4 - 2.4 GHz
	.33M	500	8252	163.5	4 – 2.4 GHz

Turbulent Flow (RANS) and Chemical Species Transport in 2D Prototype Airport



Turbulent Flow (Const. coeff. LES) and Chemical Transport in 3D Prototype Airport

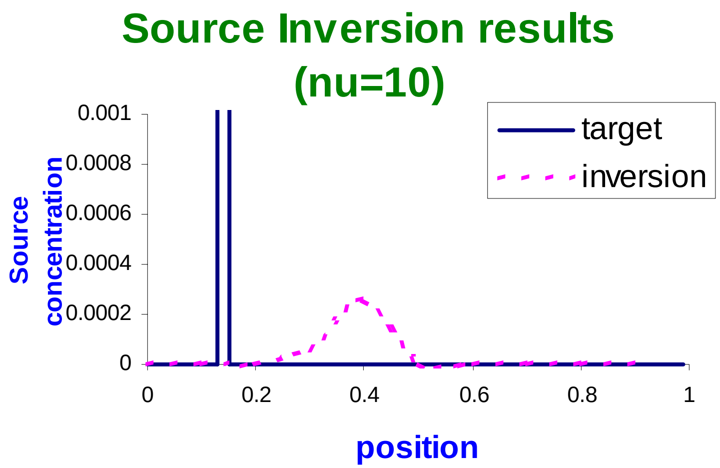


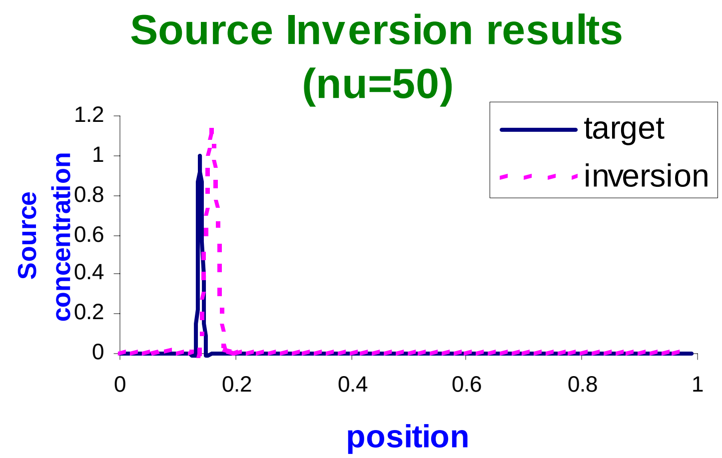
rSQP – Uses a precomputed flow field (could approx. actual conditions or ROM techniques) and optimizes inversion parameters (source locations) for given sensor readings.

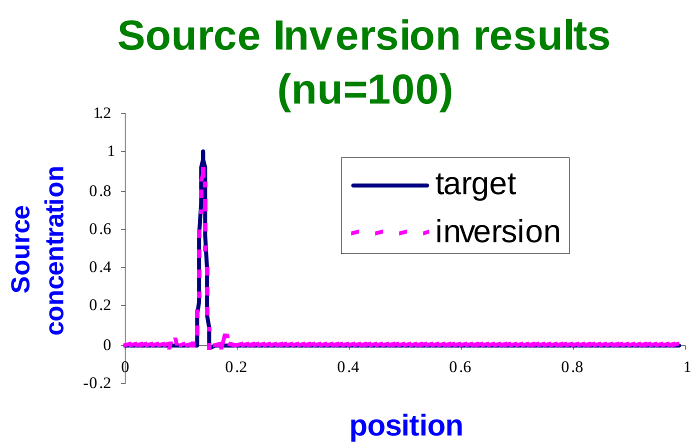
Precomputed direct sensitivities – Assumes inversion model (flow conditions in forward and inverse problem are the same) and pre-calculates direct sensitivity matrix and then solves for optimal inversion parameters (source locations) for given sensor readings.

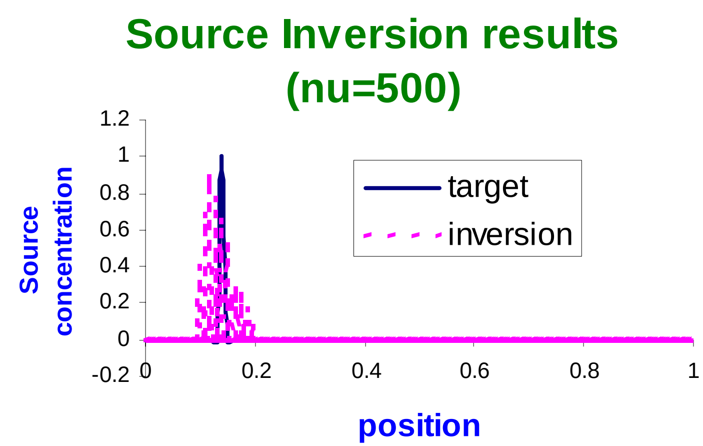
100 sensors – Next study accuracy and robustness of inversion with fewer sensors. Preliminary simulation with error in sensors (Collaborators - Boggs, Long)

Source Inversion Results: 3D Airport Terminal









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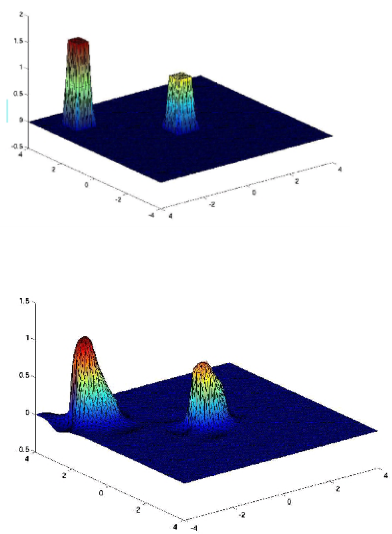
Full Space Source Inversion
Peclet Number & Time Dependence (leveraged collaborations)

Target

Total Variation



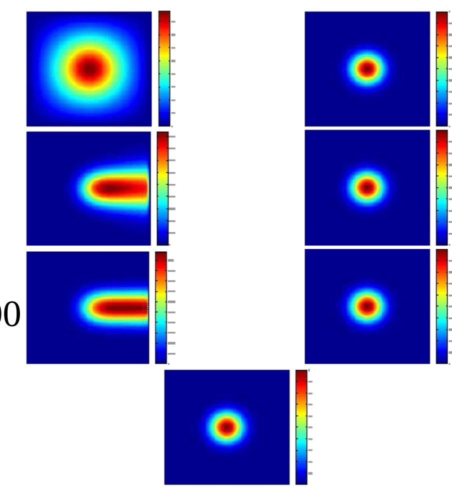
Peclet variation

inversion results

Pe=0

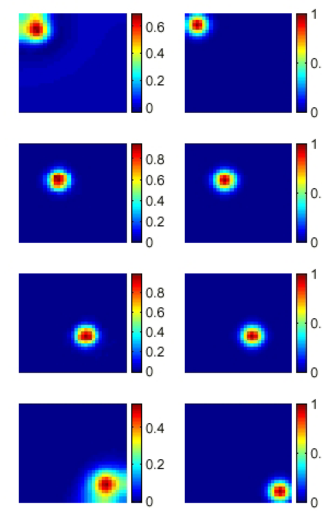
Pe=10

Pe=100



target

inversion target



moving source

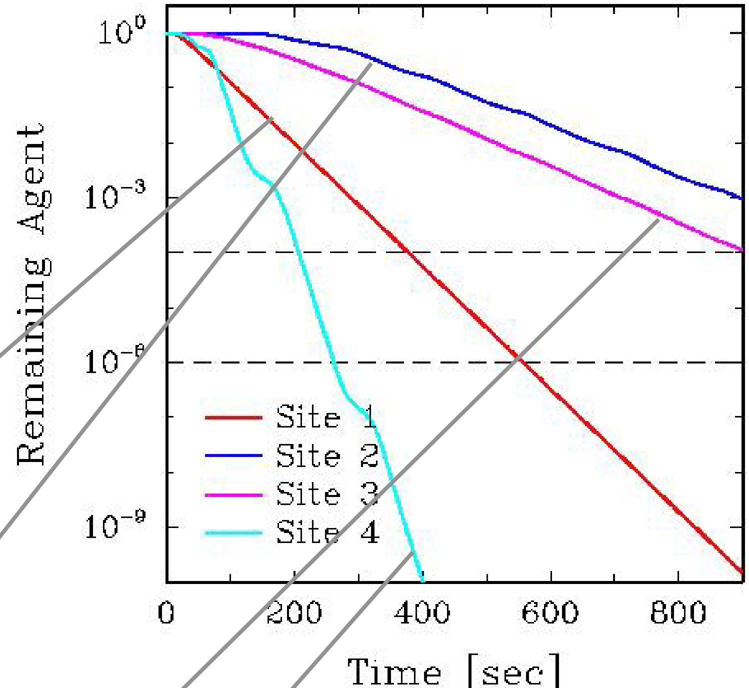
Full space approach using Newton method allows very large inversion space.
16 sensors, 40x40 mesh of concentrations and inversion parameters

* “A Variational Finite Element Method for Source Inversion for Convective Diffusive Transport”, V. Akcelik, G. Biros, O. Ghattas, K. Long, B. van Bloemen Waanders, Finite Elements In Analysis and Design 39 (8) p 683-705 2003

Preliminary Decontamination Simulation: Transient Infusion of $Cl0_2$, H_2O to Neutralize Anthrax (leveraged collaborations)

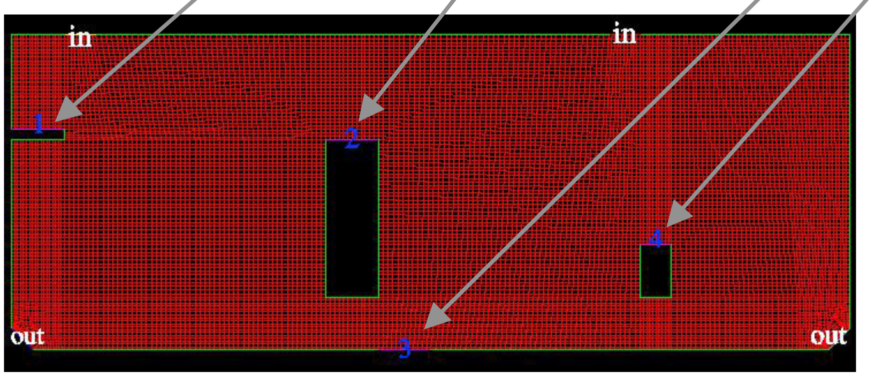
Model Info:

- **Inlets Above – ClO_2, H_20 and Air are pumped in**
- **Outlets below in Corners (Collection Hoses) – gas mixture is taken out**
- **Simplified phenomenological model for Anthrax Neutralization (not validated)**

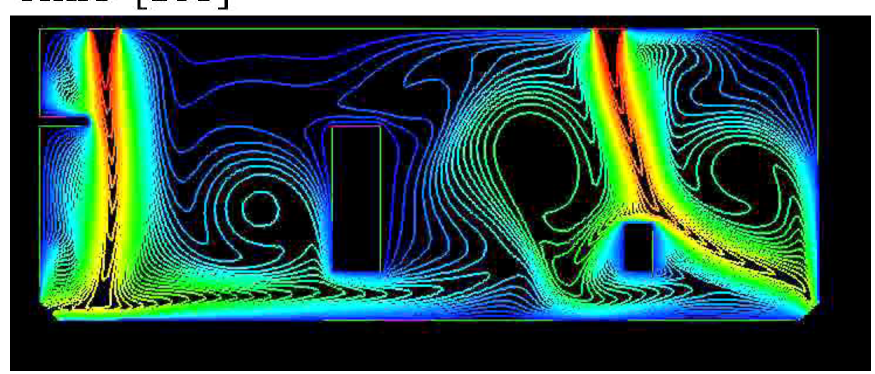


Remaining Agent: $x_i(t=0) = 1.0$

$$\boxed{dx_i/dt = k(C_{ClO2},C_{H2O})\ x}$$



Mesh & Boundary Conditions



$Cl0_2$ Concentration

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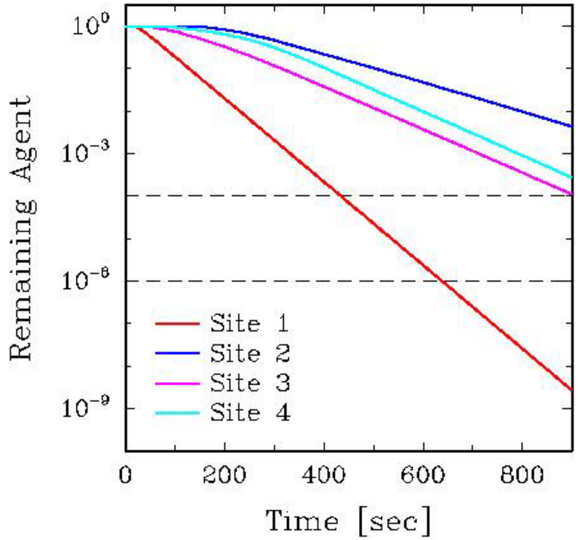
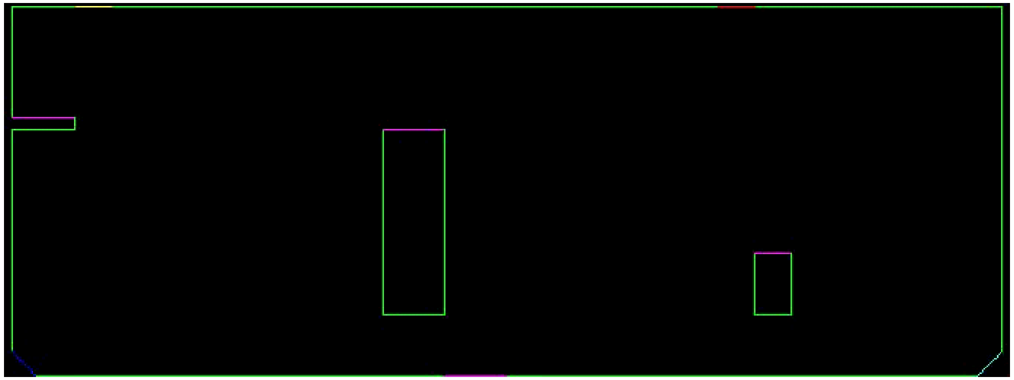
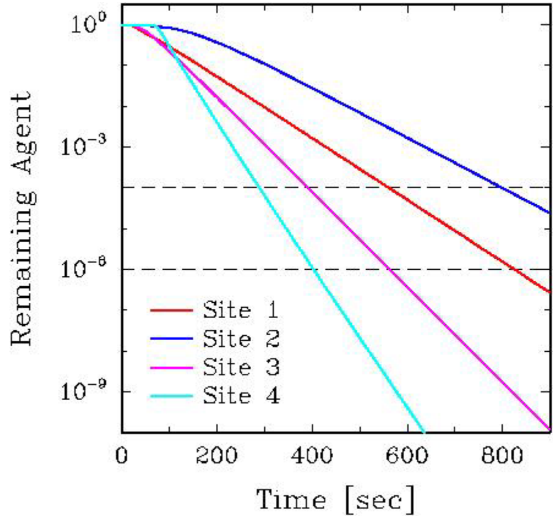
Initial vs Optimal Decontamination Procedure.

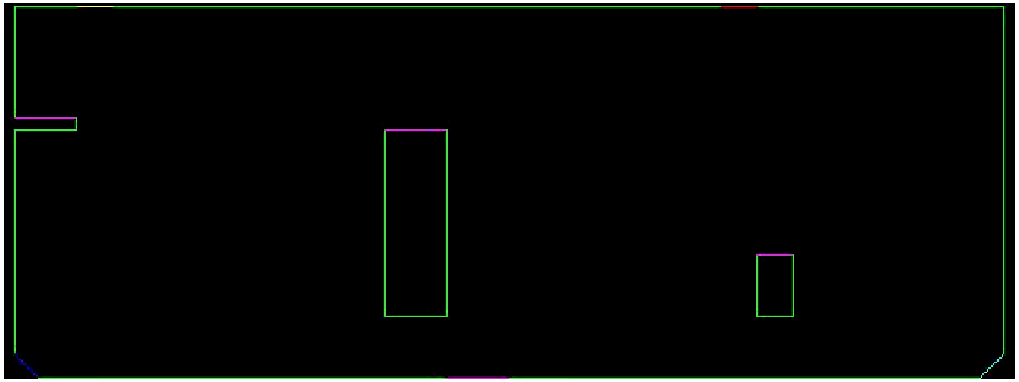


4 Optimization Parameters:
Inlet flow ratio, Outlet flow ratio
Inlet 1 angle, Inlet 2 angle

Objective Function
$F=\log[\Sigma_i x_i(t=900s)]$





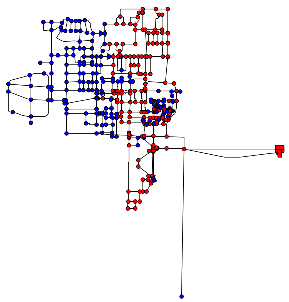


$Cl0_2$ Concentration

Leveraged Research, Development and Collaborations Supporting DHS Work

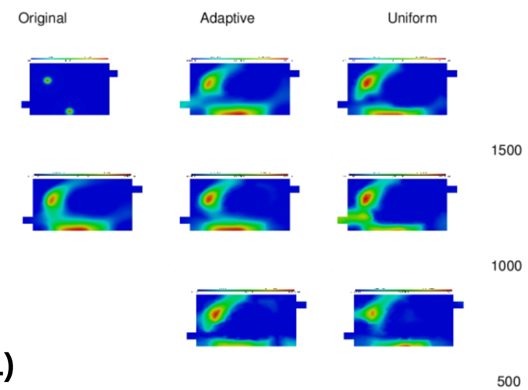
Leveraged Efforts:

SNL – Water and air security LDRD
Van Bloemen Waanders, Bartlett, Lin, Shadid, Salinger, Boggs, Long, Phillips, Hart, McKenna, Tidwell, Watson, Finley.
(network models, inversion, control, continuous & discrete optimization)



EPA -- Water security
Van Bloemen Waanders, Bartlett, Phillips, Hart McKenna, Tidwell, Watson, Finley.
(discrete and continuous optimization and network modeling)

SNL -- Rapid source inversion - Boggs, Long (reduced models – grid adaptivity)



Leveraged Collaborations:

DHS:
Restoration Domestic Demonstration Application Project (DDAP)
(Decontamination and restoration of major transportation facilities)
PIs – Imbro (LLNL), Lindner (SNL), Contact – Richard Griffiths (SNL)

NARAC - Atmospheric release/dispersion (transport / Inversion)
Contact - Gayle Sugiyama (LLNL - NARAC)

NSF ITR
Real time optimization algorithms. Biegler (CMU), Ghattas (CMU), Heinkenschloss (Rice), Keyes (Columbia), Van Bloemen Waanders (SNL)

Reduce Order Modeling
Max Gunzburger (Fl. St.)

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Major Next Steps – Project Plan

	03	04	05	06
Initial large-scale steady and transient transport and steady inversion demonstrations	X	X		
Steady transport/inversion with steady RANS and time averaged LES flow velocity 3D airport prototype		X	X	
Initial transient source inversion capabilities and Forward modeling ROM techniques.			X	
Develop initial optimal sensor placement strategies			X	
Develop and demonstrate transient inversion capabilities for an actual airport facility				X

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THE END